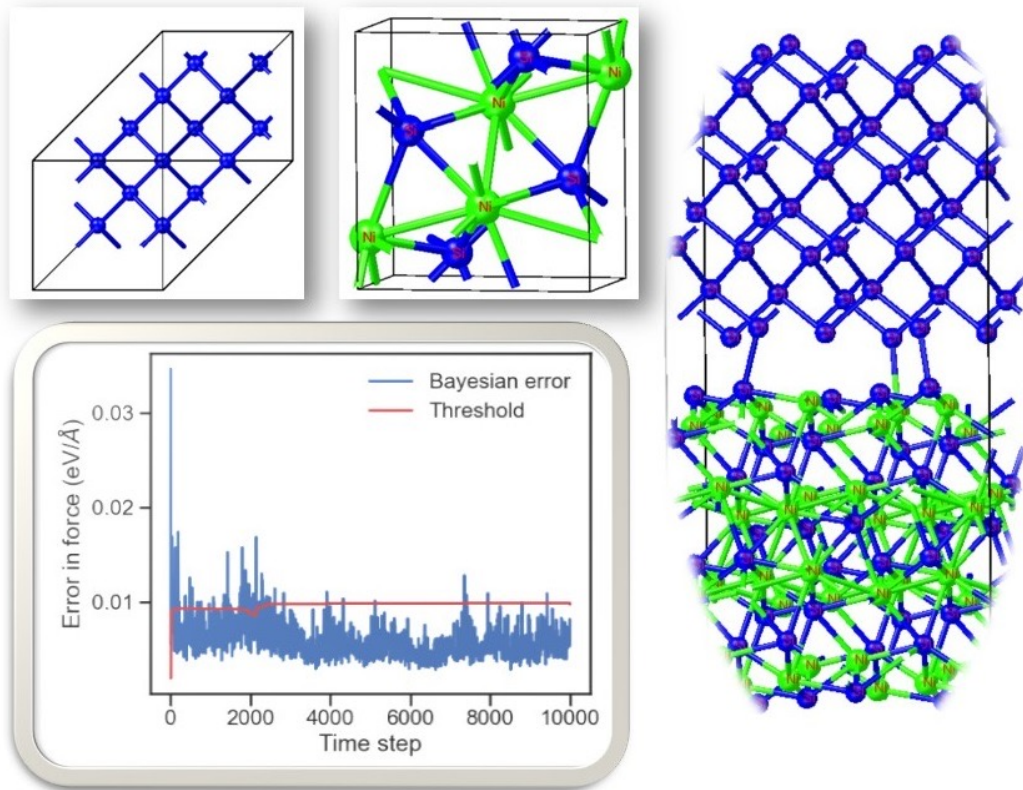


On-the-fly Machine Learning Forcefields with *MedeA VASP*

Shubham Pandey and Xiaoli Liu

Materials Design, Inc.

20th October 2022





Materials Design UGM

UGM 2022

The Materials Design annual user event will be online for 2022.

Plenary Speakers include:

Prof. Jeffrey Grossman

Prof. Georg Kresse

Dr. Carla Verdi

Prof. Jörg Behler

Dr. Jozef Bicerano



<https://ugm.materialsdesign.com/>

Materials Design UGM Training Series

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<https://www.ugm.materialsdesign.com>

- We will be recording this session

- Upcoming sessions are posted on the UGM site

- Watch any of our earlier webinars anytime www.materialsdesign.com/webinars

- Brief survey

- Take a 2 minutes brief survey at the end of the webinar

- Audio issues

- Log out and log back in again

- Check your audio output

- Google Chrome (most recent 2 versions) Mozilla Firefox (most recent 2 versions) Apple Safari (most recent 2 versions) Microsoft Edge (most recent 2 versions)



Training & Support Team

Xiaoli Liu
Presenter

Shubham Pandey
Presenter

René Windiks

Thomas Nilson

Garrett Tow

David Reith
Moderator

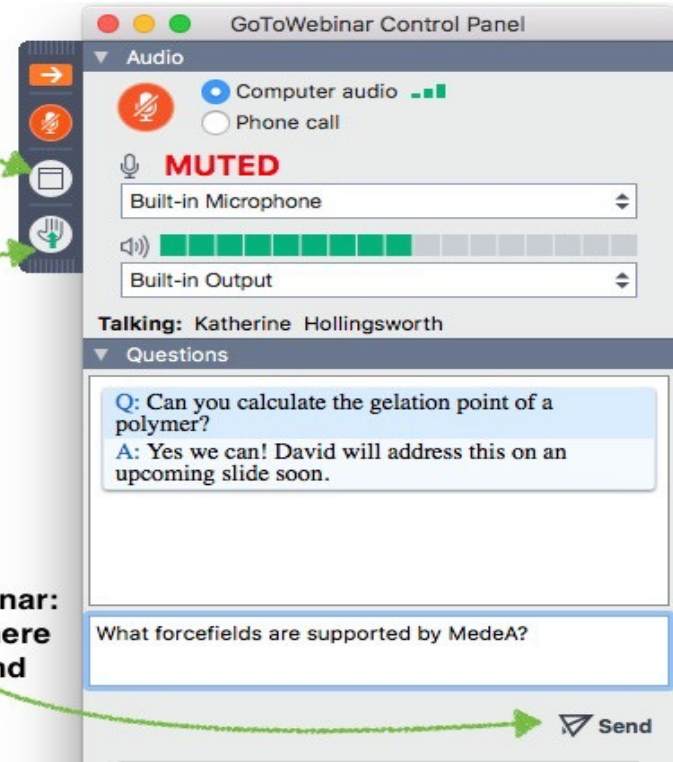
Please Ask Questions!

full screen

during discussion:
raise hand
to speak

Use the raise hand icon to bring
attention to your question

any time during webinar:
type your question here
and then press Send

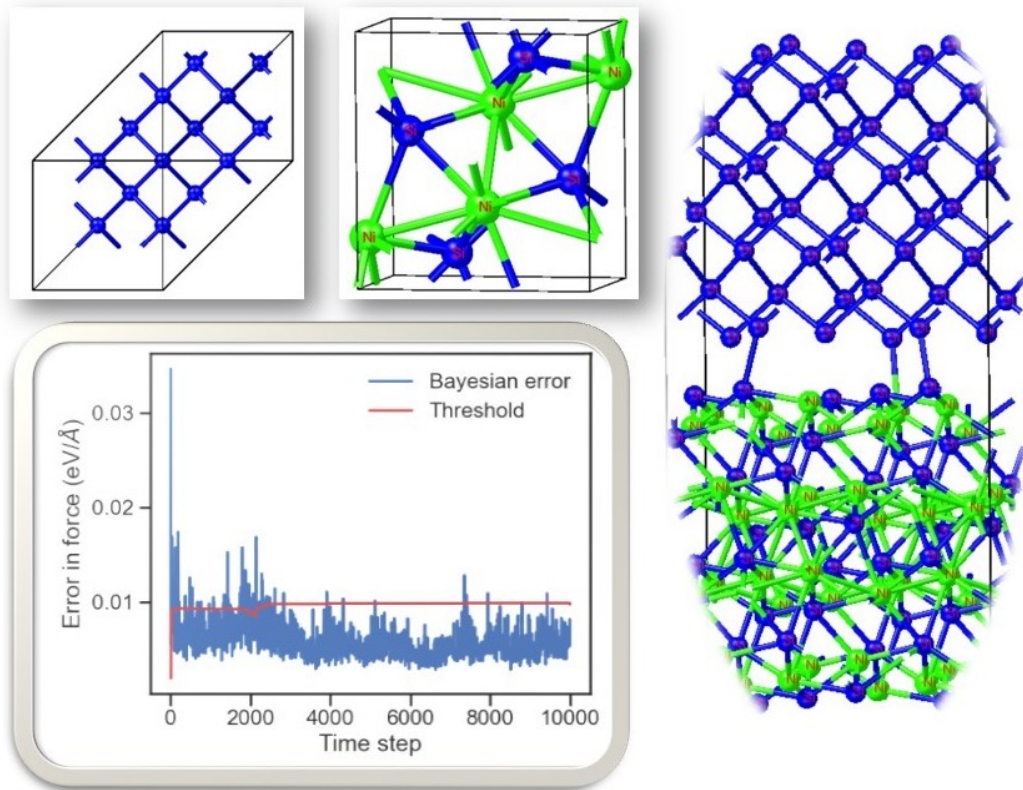


On-the-fly Machine Learning Forcefields with *MedeA VASP*

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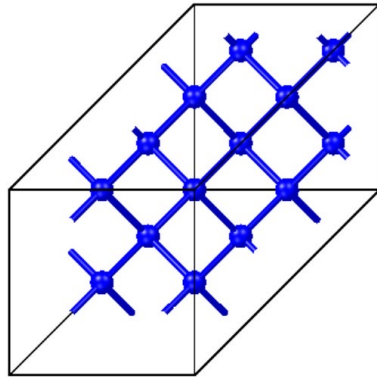
Outline

- Motivation
- MLFF basic principles
- Training MLFFs for Si, NiSi, and Si/NiSi interface
 - MLFF quality with Bayesian error and RMSE analysis
- Applying MLFF to predict volume-energy curve, thermal expansion coefficient
- Long MD simulation of Si/NiSi interface with MLFF
- Guidelines for MLFF training

Ab-initio Molecular Dynamics

- Ab-initio MD traditionally used to accurately determine dynamic properties of materials
- Interactions of atoms and electrons are calculated fully quantum-mechanically
- Limited to small simulation times (few ps) and small cells (few 100 atoms)
- One of the workarounds: machine-learned forcefields to dramatically accelerate these calculations

Pure Si, 16 atoms



nPT, 2fs timestep, 400K, 12 CPU cores

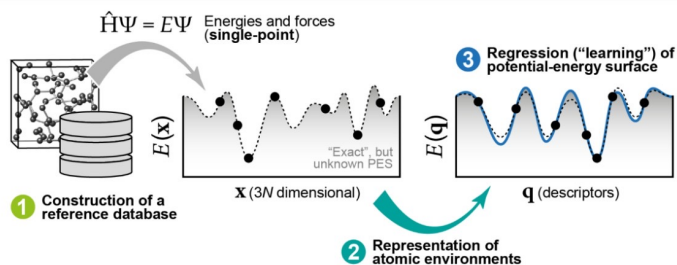
- 3ps VASP-MD: 32 min
- 20ps MLFF-MD: 1.6 min

Key steps of machine-learning

Step-1: training data generation (“on-the-fly”)

Step-2: feature selection (representation of local environment)

Step-3: ML model selection (such as neural network or a regression method)



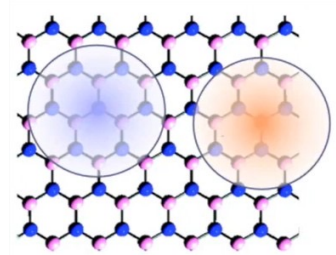
Database \rightarrow Features \rightarrow Regression

Deringer et al., *Adv. Mater.* 31, 1902765 (2019)

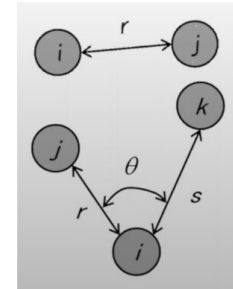
Features and regression model

Database → Feature → Regression

- Combination of pair-correlation and angular functions
 - $\rho^1(r) = g(r)$
 - $\rho^2(r, s, \theta)$
- Likelihood of finding of one particle at distance r , and another at s at an angle θ
- Both are translationally and rotationally invariant
- Total energy is then a function of local environment dependent local energies (just an approximation – DFT does not break up the energies into local energies!)
- Kernel regression to approximate the total energy function
- $E = \sum_i^{N_a} \sum_{i_B} K(x_i, x_{i_B}) w_{i_B}$
- “reference atoms” are chosen from the entire dataset and fitting weights are determined for those reference atoms to obtain an approximation of the total energy



Classical density distribution of atoms around a central atom



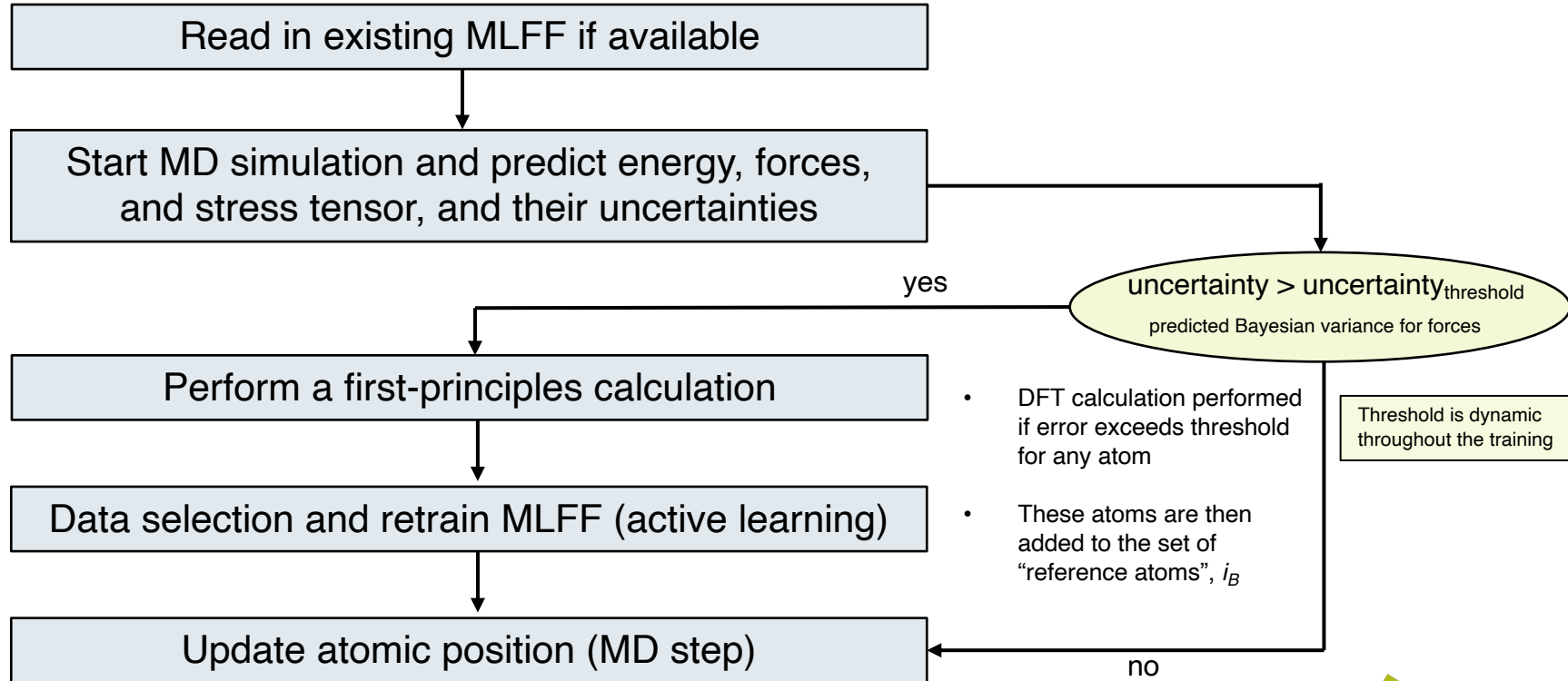
Pair-correlation and angular functions


Jinnouchi et al., *J. Chem. Phys.* 152, 234102 (2020)

How do we choose training set structures and those reference atoms?

On-the-fly machine-learning

Database → Descriptors → Regression

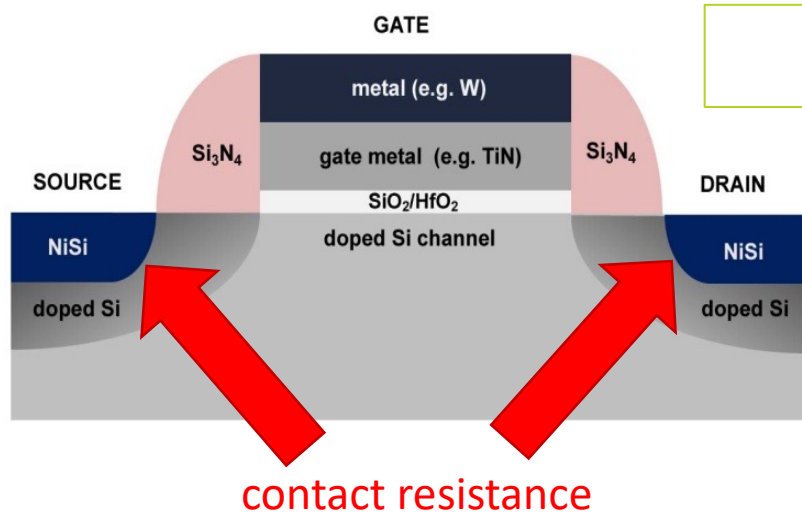




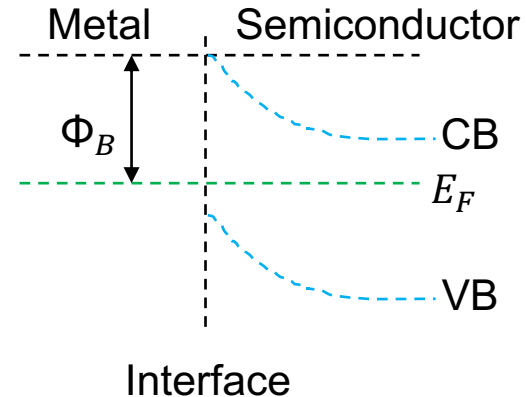
MLFF for Si, NiSi, and Si/NiSi Interface: motivation

NiSi/Si interface in CMOS device

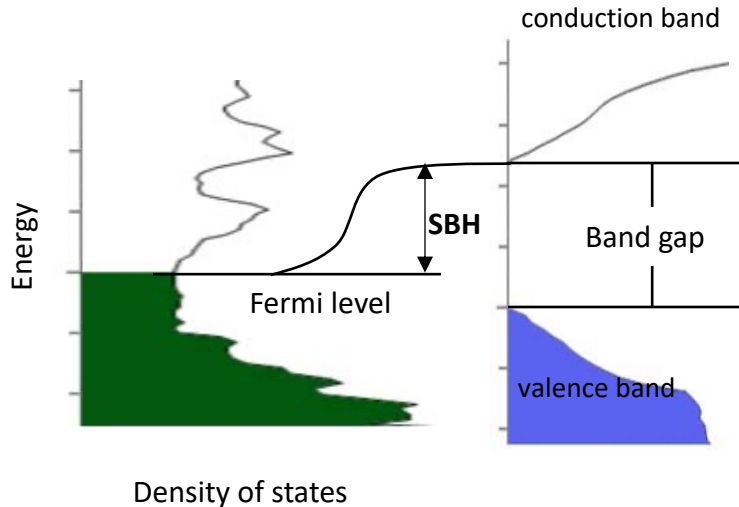
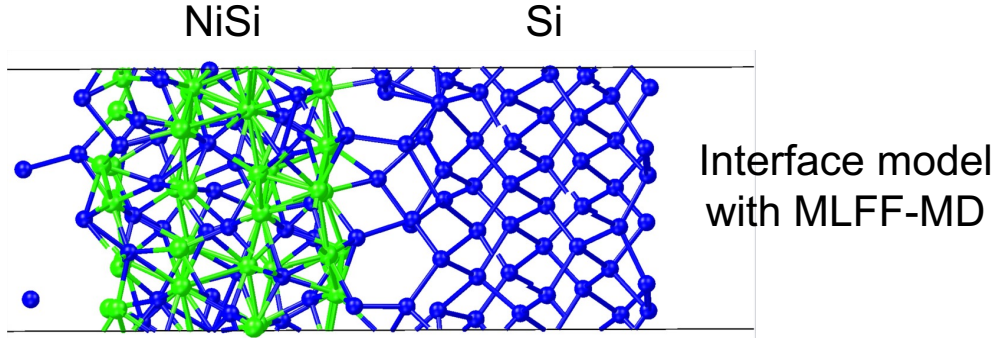
NiSi is commonly used in complementary metal oxide semiconductor (CMOS) devices because its workfunction can be adjusted. The contact resistance at the source and drain remains a critical bottleneck, which is controlled by the Schottky barrier (SB) at the interface between the metallic NiSi and semiconducting Si regions.



$$J \propto e^{\frac{kT}{SBH}} \cdot \left(e^{\frac{qV}{kT}} - 1 \right)$$



Possible application of the NiSi/Si interface structure

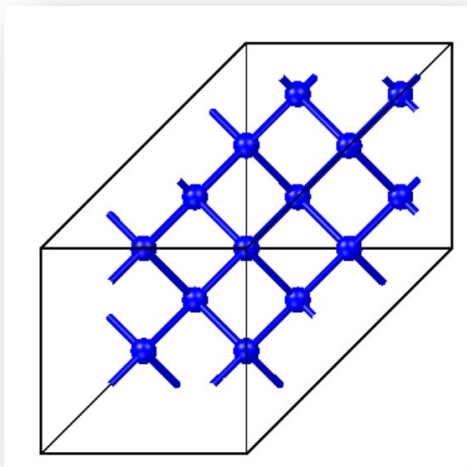


DOS alignment to predict SBH

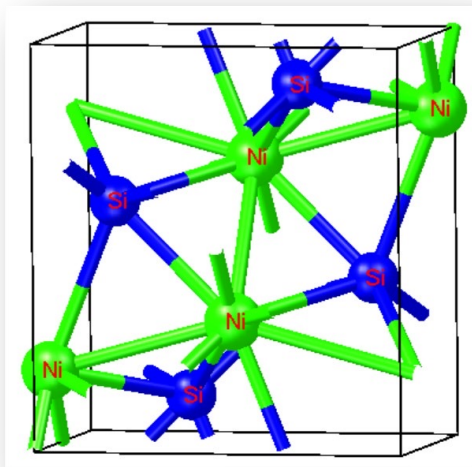
What can MLFF do?

- ▶ Accelerate VASP-MD calculation
- ▶ Calculate for a larger system
- ▶ Longer simulation time (e.g., 20 ps)
- ▶ ...

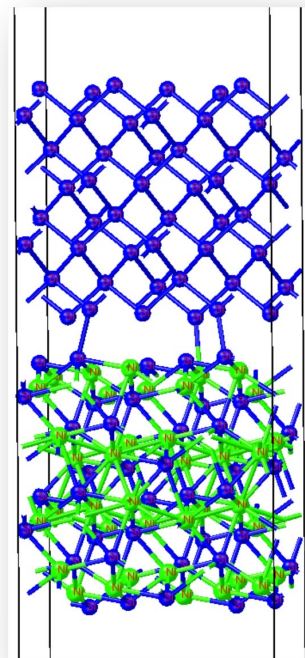
Material systems of interest: Si, NiSi, Si/NiSi interface



MLFF-1: Si



MLFF-2: Si & NiSi, Pnma, s.g. #62 (bulk)

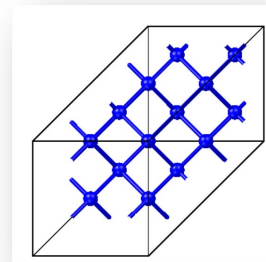


MLFF-3: Si & NiSi (bulk)
& Si/NiSi(100) interface

- Step-1: train an MLFF on pure Si only
- Step-2: train an MLFF on NiSi starting from MLFF created in step-1
- Step-3: finally, train an MLFF on Si/NiSi interface starting from MLFF created in step-2

MLFF for pure Si

Setting-up MLFF training with MedeA VASP



MedeA - - [(Si)₁₆ (P1) ~ Si16 -- Job 68020 initial: Si-VASP-MD-NPT-3ps]

File Edit Builders Tools Jobs Forcefields InfoMaticA VASP 6 Analysis Windows Help

Run

Band Structure: Run a simulation on the current system

MedeA : Run VASP 6

Calculation Functional/Potential SCF DOS/Optic/Tensors Band Structure Advanced/Restart Add to Input Preview Input

Type of calculation: Molecular Dynamics

Molecular Dynamics Parameters

Ensemble: isothermal-isobaric (nPT)

Simulation time: 20000 fs

Time step: 2.0 fs

Trajectory file frequency: 1 steps

Temperature initial: 400.0 K

Temperature end: K

Parrinello-Rahman mass:

Continuation of job: ...

Involve machine-learned forcefield

Task: Create forcefield by on-the-fly learning

Properties

(Pseudo, difference, spin) charge density

Total local potential

Electron localization function

Wave functions

Electric field gradients

Hyperfine parameters

Work function (surfaces only)

(Total, valence) charge density, Bader analysis

Band structure

Density of states

Optical spectra

Zone center phonons

Response tensors

NMR: chemical shifts

Energy of formation

Solvation (for molecules or surfaces)

Apply solvation model

External pressure: 0 GPa

Charge state: 0 e

External electrostatic field (molecules and surfaces): none

Interaction

Functional: Density functional

DFT exchange-correlation: GGA-PBE

Van der Waals: DFT-D2 forcefield (Grimme)

Magnetism: Defined by model (to be non-magnetic)

General Setup

Precision: Normal

Increase planewave cutoff (cell optimizations)

Planewave cutoff (default): 318.949 eV

Planewave cutoff: eV

Projection: Reciprocal space

VASP version: standard

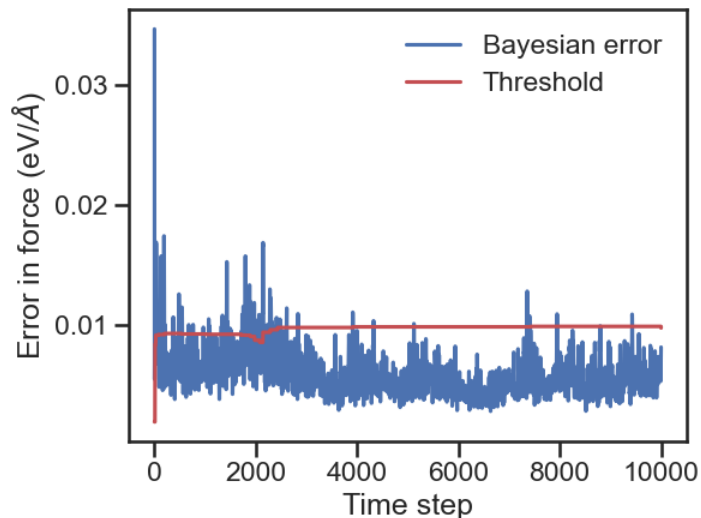
Title: (Si)₁₆ (P1) ~ Si16 (VASP)

Run Close Write input files Restore defaults Restore from job

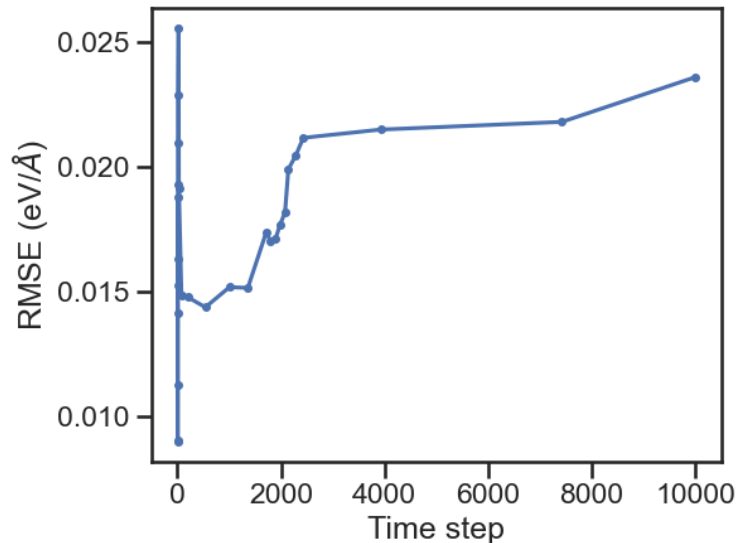
- VASP 6 GUI
- Type of calculation: Molecular Dynamics
- nPT Ensemble
- 10,000 time-steps
- Elevated temperature
- Involve machine-learned forcefield

(1) Pure Si - Bayesian error and RMSE on atomic forces

Bayesian error on maximum of all forces on atoms (an estimate of *out-of-sample* error)



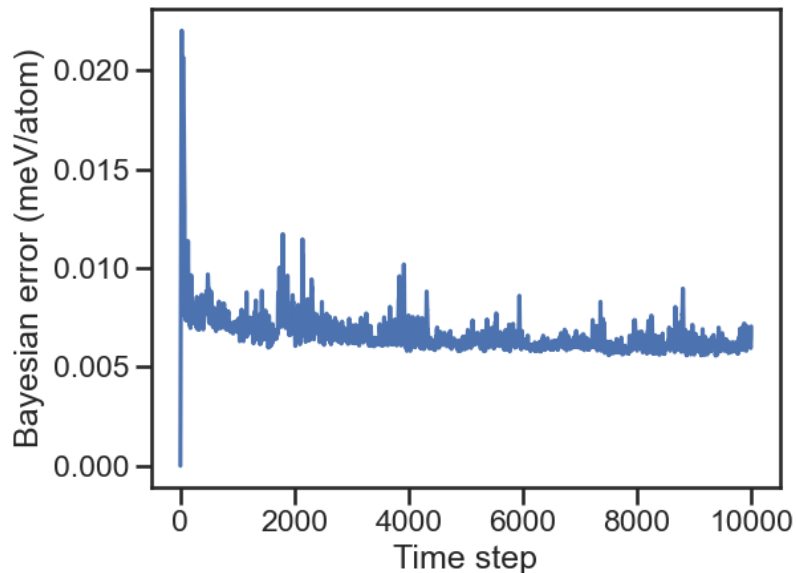
RMSE of forces w.r.t ab-initio data (real error on training structures up to the step where FF is updated)



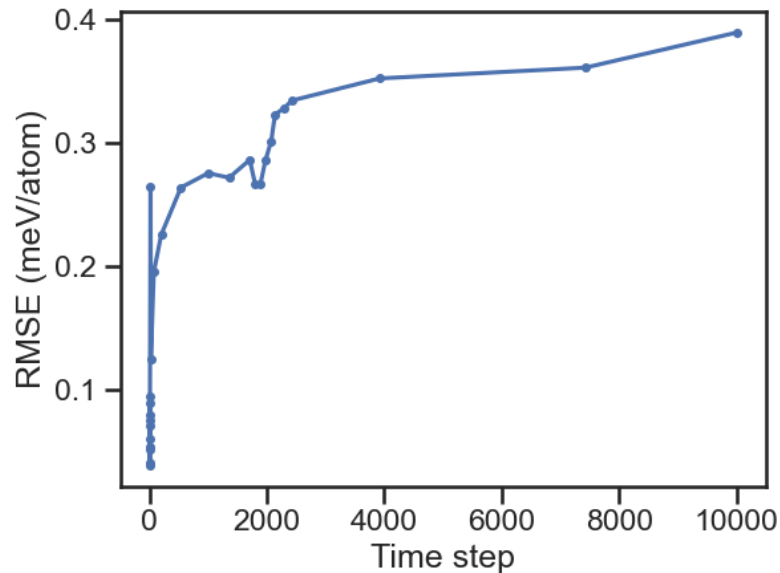
- Bayesian error catches error in the data but retaining error in the probability model
- Fluctuations in Bayesian error go down with increasing MD steps
- Sudden fluctuation at an MD step indicates a local configuration of atoms encountered by forcefield far away from what VASP has learned
- Training time: ~23 min, 16 atoms, 20 ps, 12 cores
- **Good accuracy: 0.03-0.1 eV/Å for temperatures 300-1000 K**

(1) Pure Si - Bayesian error and RMSE on total energies

Bayesian error of energy per atom



RMSE of energy per atom



Good accuracy: <5 meV/atom for temperatures 300-1000 K

How to use MLFF for property calculations?

MedeA - - [(Si)₁₆ (P1) ~ Si16 -- Job 68020 initial: Si-VASP-MD-NPT-3ps]

File Edit Builders Tools Jobs Forcefields InfoMaticA VASP 6 Analysis Windows Help

Run

MedeA : Run VASP 6

Calculation Functional/Potential SCF DOS/Optic/Tensors Band Structure Advanced/Restart Add to Input Preview Input

Type of calculation Molecular Dynamics

Molecular Dynamics Parameters

Ensemble isothermal-isobaric (nPT)

Simulation time: 20000 fs

Time step: 2

Trajectory file frequency: 1

Temperature initial: 400

Temperature end:

Parrinello-Rahman mass:

Continuation of job:

Involve machine-learned forcefield

Task Create forcefield by on-the-fly learning

Properties

(Pseudo, difference, spin) charge density

Total local potential

Electron localization function

(Total, valence) charge density, Bader analysis

Band structure

Density of states

Interaction

Functional Density functional

DFT exchange-correlation GGA-PBE

Van der Waals DFT-D2 forcefield (Grimme)

Defined by model

to be non-magnetic

Normal

ff (cell optimizations)

Plane wave cutoff (default): 318.949 eV

Plane wave cutoff:

Projection Reciprocal space

VASP version standard

External pressure: 0 GPa

Charge state: 0 e

External electrostatic field (molecules and surfaces) none

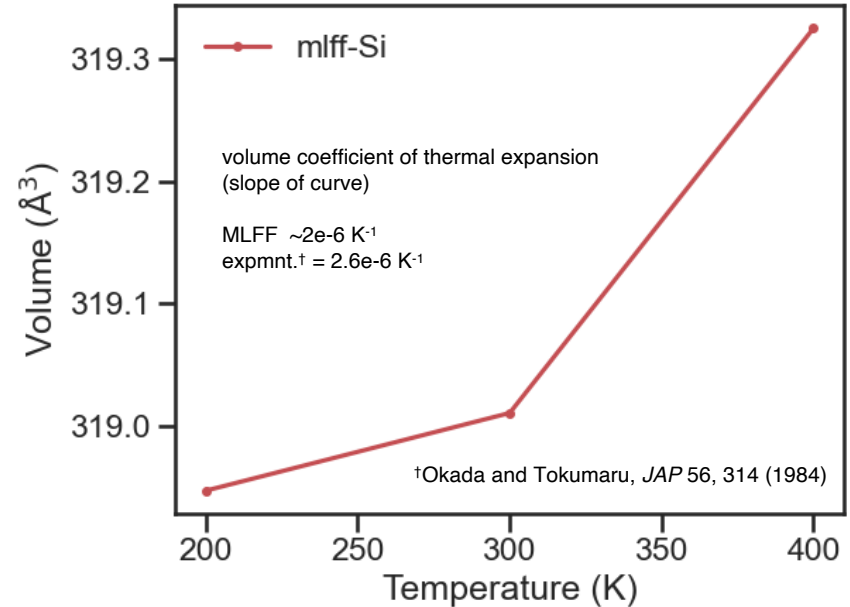
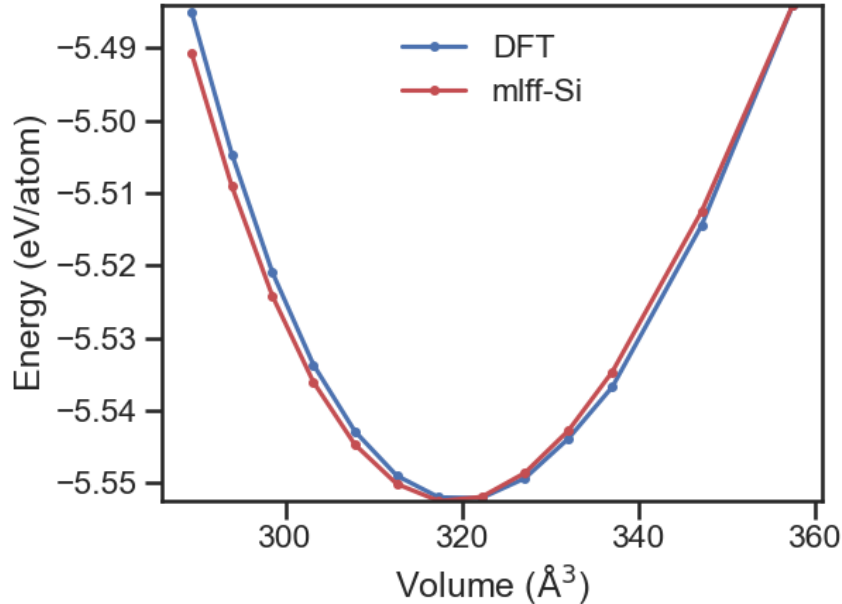
Title: (Si)₁₆ (P1) ~ Si16 (VASP)

Run Close Write input files Restore defaults Restore from job

Live Demo

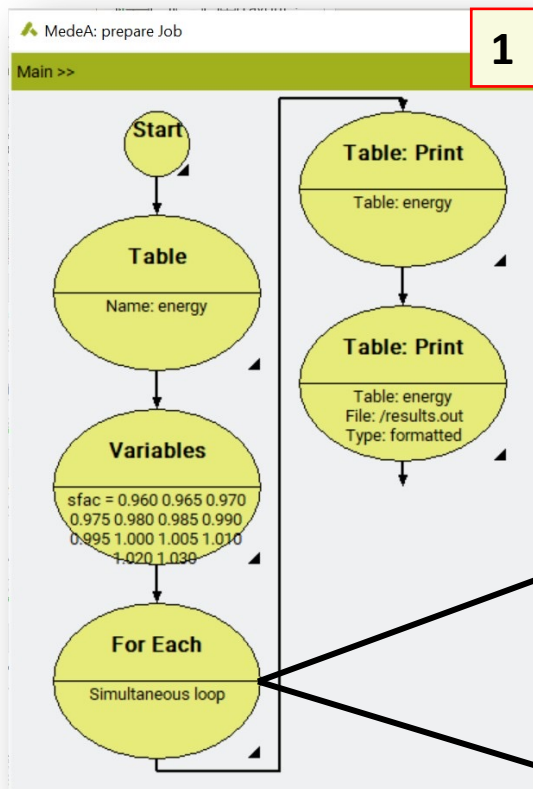
(1) Pure Si – volume-energy curve and thermal expansion

MLFF trained from scratch on Si



- Single-point calculations on expanded/contracted cells
- Good agreement between MLFF predicted lowest energy volume with DFT
- Fairly good agreement of MLFF predicted thermal expansion coefficient with experiments
- Compute time: ~ 1.6 min, 16 atoms, 20 ps, 12 cores

Apply trained MLFF for volume-energy curve



Edit stage: VASP 6

3

Calculation Functional/Potential SCF DOS/Optic/Tensors Band Structure Advanced/Restart Add to Input Preview Input

Type of calculation Molecular Dynamics

Molecular Dynamics Parameters

Ensemble micro canonical (nVE)

Simulation time: 120.0 fs

Time step: 4.0 fs

Trajectory file frequency: 1 steps

Temperature initial: 298.0 K

Continuation of job:

Involve machine-learned forcefield

Task Apply machine-learned forcefield

Using forcefield of job: 64901

Properties

(Pseudo, difference, spin) charge density

Total local potential

Electron localization function

Wave functions

Electric field gradients

Hyperfine parameters

Work function (surfaces only)

(Total, valence) charge density, Bader analysis

Band structure

Density of states

Optical spectra

Zone center phonons

Response tensors

NMR: chemical shifts

Energy of formation

Interaction

Functional Density functional

DFT exchange-correlation GGA-PBE

Van der Waals DFT-D2 forcefield (Grimme)

Magnetism Defined by model

to be non-mag

General Setup

Precision Normal

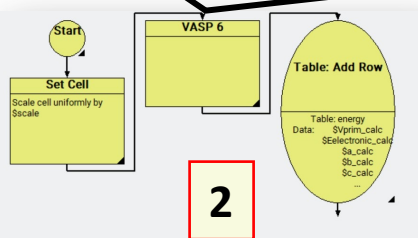
Increase plane-wave cutoff (cell optimizations)

Plane-wave cutoff (default): 269.532 eV

Plane-wave cutoff: 300 eV

Projection Reciprocal space

VASP version standard



Edit stage: VASP 6

4

Calculation Functional/Potential SCF DOS/Optic/Tensors Band Structure Advanced/Restart Input added Preview Input

Additional Input Lines

```
Begin input file: INCAR
IBRION = 2
NSW = 1
ISIF = 3
ML_IMLFF = T
ML_ISTART = 2
End input file: INCAR
```

Apply trained MLFF for thermal expansion

3 different calculations for 200 K, 300 K, 400 K

MedeA: prepare Job

Main

1

Start

VASP 6

VASP 6

VASP 6

Edit stage: VASP 6

2

Calculation Functional/Potential SCF DOS/Optic/Tensors Band Structure Advanced/Restart Add to Input Preview Input

Type of calculation Molecular Dynamics

Molecular Dynamics Parameters

Ensemble isothermal-isobaric (nPT)

Simulation time: 20000 fs

Time step: 2.0 fs

Trajectory file frequency: 100 step

Temperature initial: 400.0 K

Temperature end: K

Parrinello-Rahman mass:

Continuation of job:

3

✓ Involve machine-learned forcefield

Task Apply machine-learned forcefield

Using forcefield of job: 65378

4

JobServer Home Summary Jobs Administration Documentation

./Stage_1/REPORT output for 64991: MLFF-Si-tutorial-3-ensemble-avg-lattice-p

Status: finished

```

IDALGO = 3
LANGEVIN_GAMMA = 1.000
LANGEVIN_GAMMA_L = 10.000
SCALING = 0
CNEXP = 9.000 14.000
PHASS = 10.00000
LATTICE_CONSTRAINTS = T T T (X,Y,Z) = 9 degree(s) of freedom
RANDOM_SEED = 311157787

original number of atomic DOF: 48
number of independent constraints: 0
number of active DOF: 48

=====
ND step No. 1
=====
Atomic velocities initialized by STEP_tb
>Monit_coord
m> LR 7.71854
m> LR 7.70825
m> LR 7.58820
m> LA 1.06353
m> LA 1.04928
m> LA 1.03577
m> LV 319.41623

Lattice velocities initialized by STEP_tb
t_b> 300.000 307.152 237.341 296.098

>Energies
e_b> -0.87246585E+02 E_tot E_pot E_kin EPS ES
0.00000000E+00 -0.87937387E+02 0.72720241E+00 0.00000000E+00
                    
```

Add to Input: ICONST

Edit stage: VASP 6

3

Calculation Functional/Potential SCF DOS/Optic/Tensors Band Structure Advanced/Restart Input added Preview Input

Additional Input Lines

Begin input file: ICONST

LR 1 7 } Monitor length of lattice vectors

LR 2 7 }

LR 3 7 }

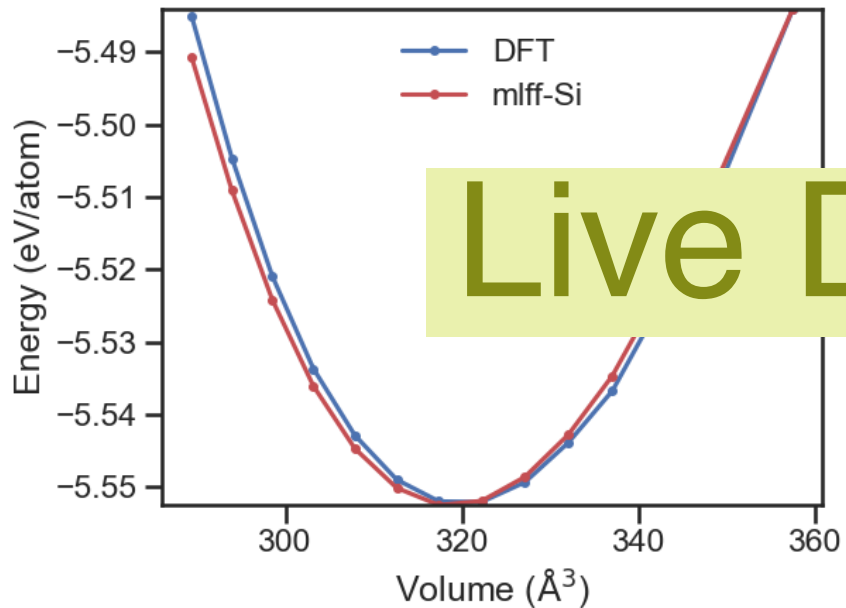
LA 2 3 7 } Monitor angle between lattice vectors

LA 1 3 7 }

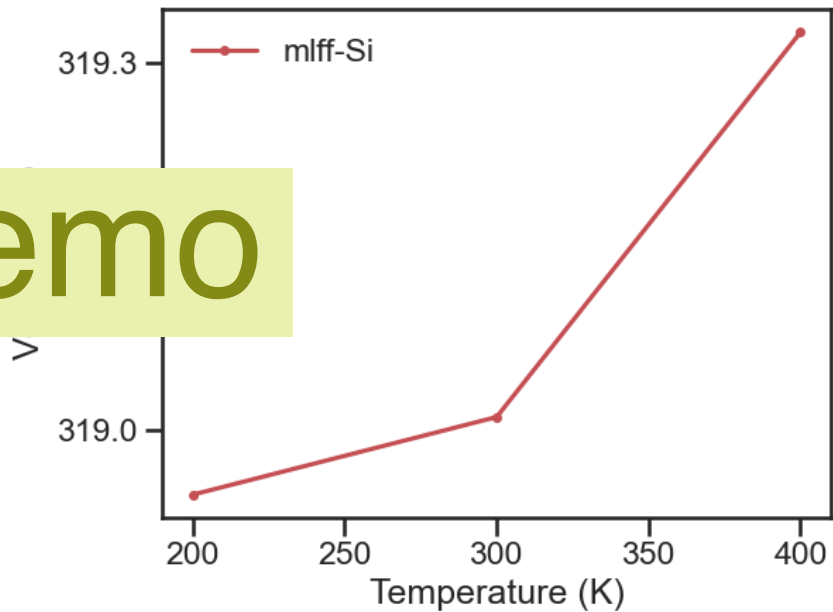
LA 1 2 7 }

LV 7 } Monitor lattice volume

End input file: ICONST

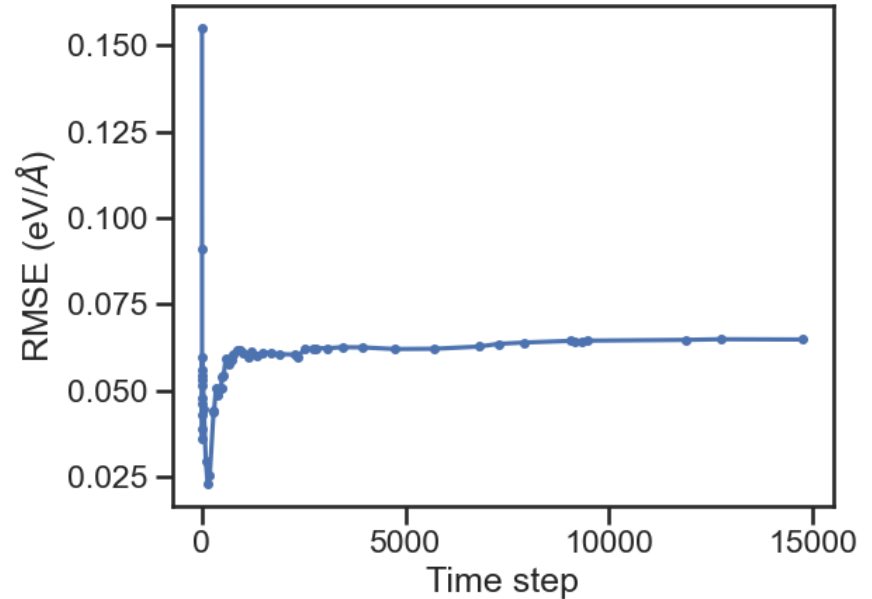
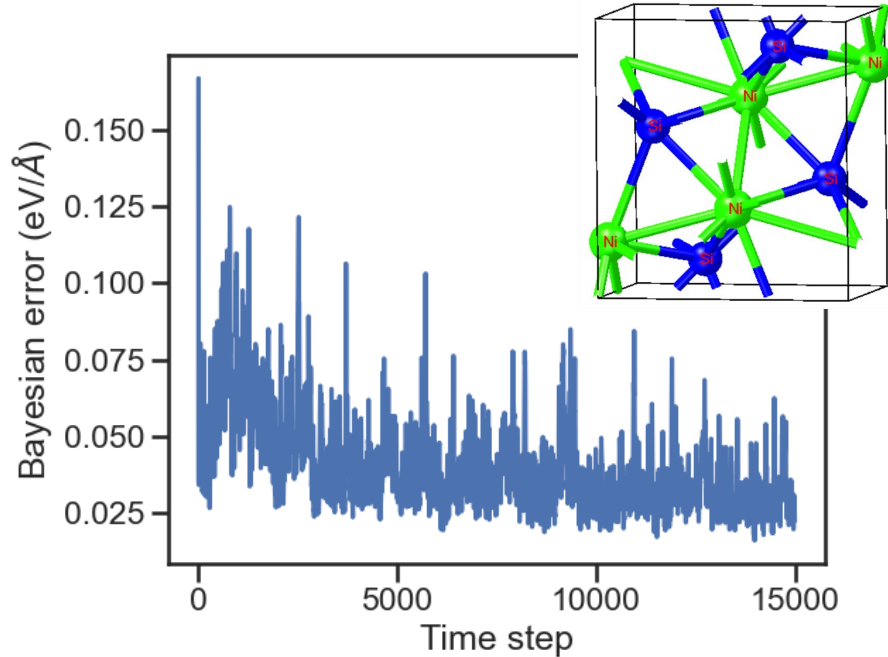


Live Demo



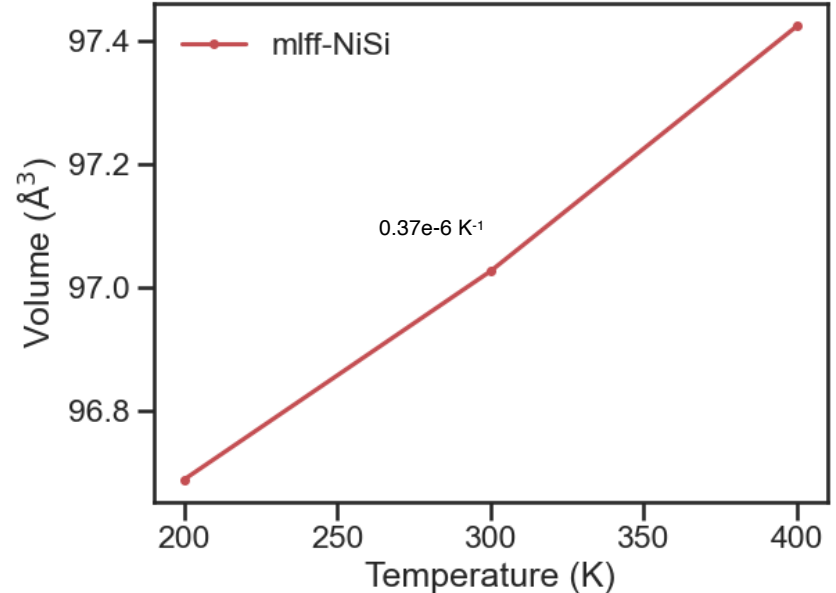
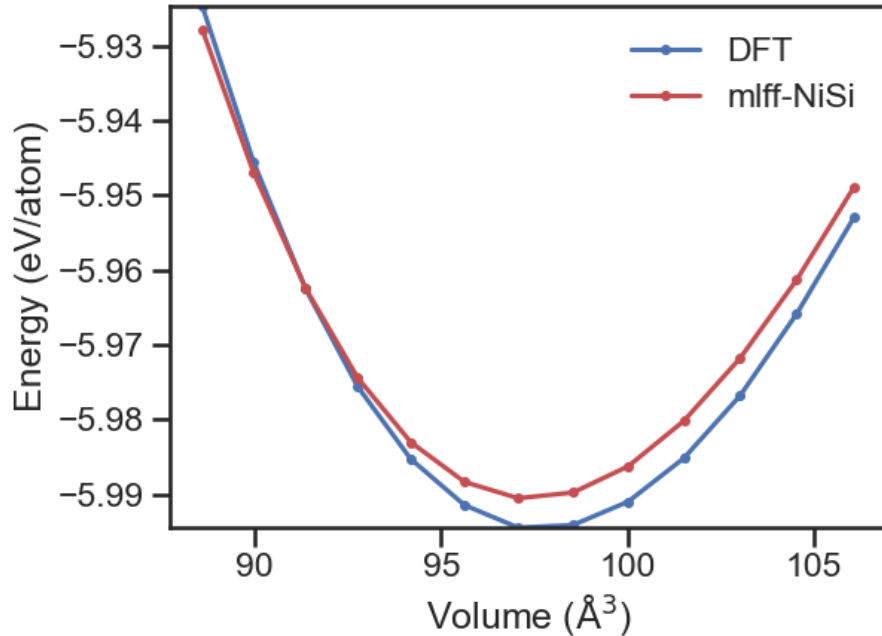
MLFF for NiSi: from scratch and
starting from pretrained Si MLFF

(2) Pure NiSi: train an MLFF on NiSi *from scratch*



- 30ps, 400 K, nPT, unit cell used
- Acceptable accuracy on forces (<100 meV/Å)
- Improve fluctuations: more accurate DFT settings, supercell instead of unit cell
- Training time: ~45min, 8 atoms, 30 ps, 12 cores

(2) Pure NiSi – volume-energy curve and thermal expansion *MLFF trained from scratch on NiSi*



How to continue training from the pretrained MLFF on pure Si?

(2) Pure NiSi: train an MLFF on NiSi *starting from pretrained MLFF for Si*

Calculation Functional/Potential SCF DOS/Optic/Tensors Band Structure Advanced/Restart Add to Input Preview Input

Type of calculation: Molecular Dynamics

Molecular Dynamics Parameters

- Ensemble: isothermal-isobaric (nPT)
- Simulation time: 30000 fs
- Time step: 2.0 fs
- Trajectory file frequency: 1 steps
- Temperature initial: 400.0 K
- Temperature end: K
- Parrinello-Rahman mass: K

Continuation of job: ...

Involve machine-learned forcefield

Task: Continue on-the-fly learning

Using forcefield of job: 64901

Properties

- (Pseudo, difference, spin) charge density
- Total local potential
- Electron localization function
- Wave functions
- Electric field gradients
- Hyperfine parameters
- Work function (surfaces only)
- (Total, valence) charge density, Bader analysis
- Band structure
- Density of states
- Optical spectra
- Zone center phonons
- Response tensors
- NMR: chemical shifts
- Energy of formation

Solvation (for molecules or surfaces)

- Apply solvation model

External pressure: 0 GPa

Charge state: 0 e

External electrostatic field (molecules and surfaces): none

Interaction

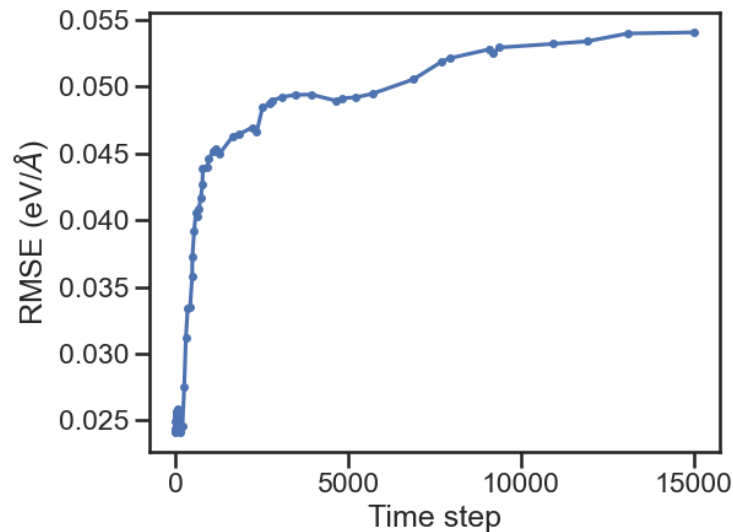
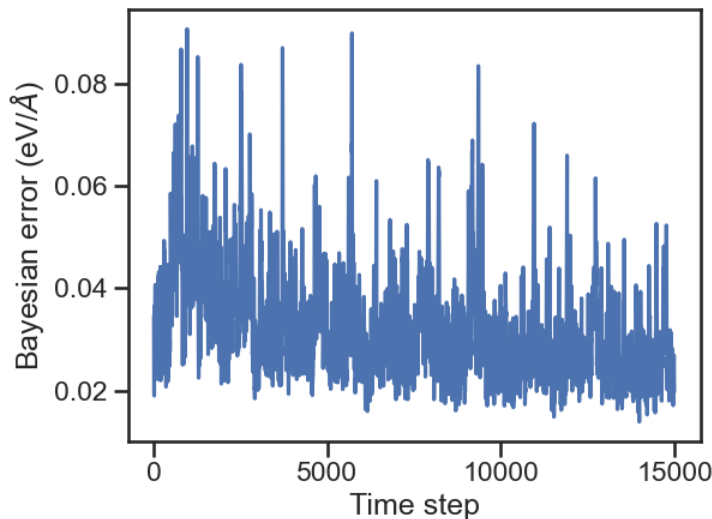
- Functional: Density functional
- DFT exchange-correlation: GGA-PBE
- Van der Waals: None
- Magnetism: Defined by model

General Setup

- Precision: Normal
- Increase planewave cutoff (cell optimizations)
- Planewave cutoff (default): 269.532 eV
- Planewave cutoff: 300 eV
- Projection: Reciprocal space
- VASP version: standard

Continue from the
MLFF trained on Si

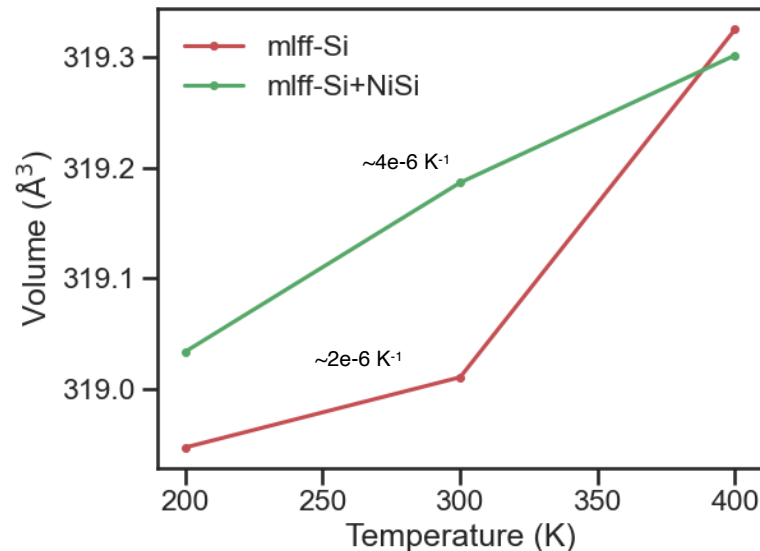
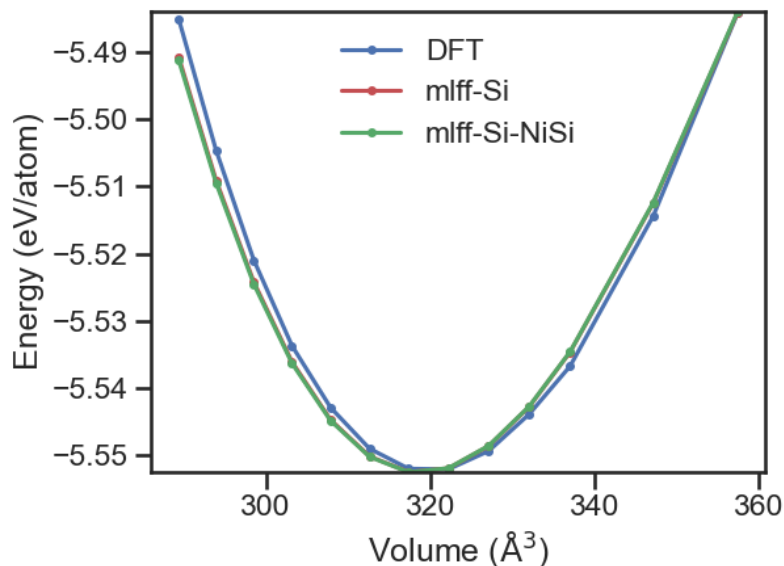
(2) Pure NiSi - Bayesian error and RMSE on atomic forces starting from MLFF of pure Si



- 30ps, 400 K, nPT, 300 eV plane-wave cutoff, 2x2x2 k-mesh, unit cell used
- Larger fluctuations than MLFF trained on NiSi from scratch, but acceptable accuracy on forces (<100 meV/Å)
- Possible solutions to minimize fluctuations and error: higher plane-wave cutoff, denser k-mesh, larger cell size
- Training time: ~ 45 min, 8 atoms, 30 ps, 12 cores

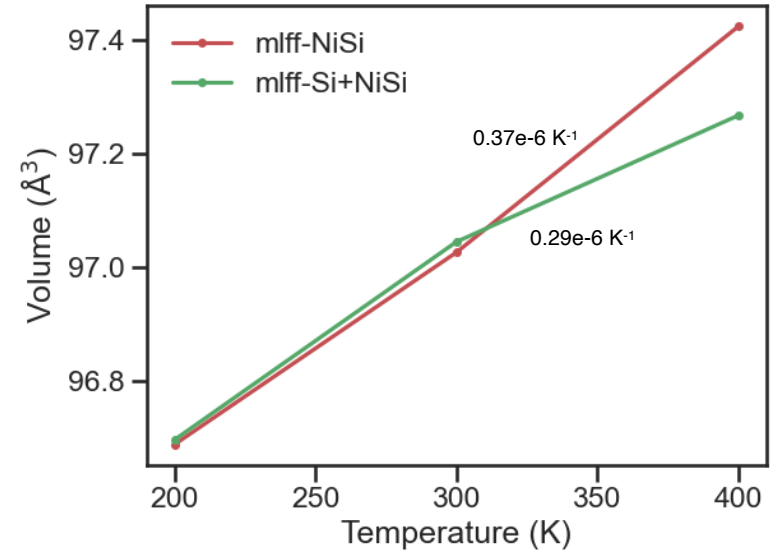
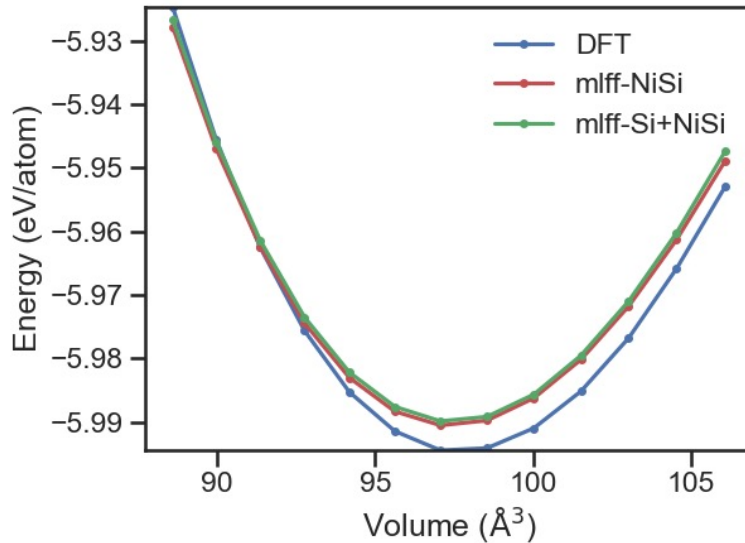
How does this combined Si+NiSi MLFF perform for Si and NiSi properties?

(1) Pure Si – volume-energy curve and thermal expansion *combined MLFF on Si+NiSi*



- MLFF trained on Si+NiSi performs equally good for volume-energy of Si, as MLFF trained on Si only
- Slight deviations between MLFF trained on Si+NiSi and Si only for thermal expansion of Si
- Compute time: ~ 11 min, 16 atoms, 20 ps, 12 cores

(2) Pure NiSi – volume-energy curve and thermal expansion combined MLFF on Si+NiSi



- MLFF trained on Si+NiSi performs equally good for volume-energy of NiSi, as MLFF trained on Si only
- Slight deviations between MLFF trained on Si+NiSi and Si only for thermal expansion of NiSi at higher temperature
- Compute time: ~18min, 8 atoms, 20 ps, 12 cores

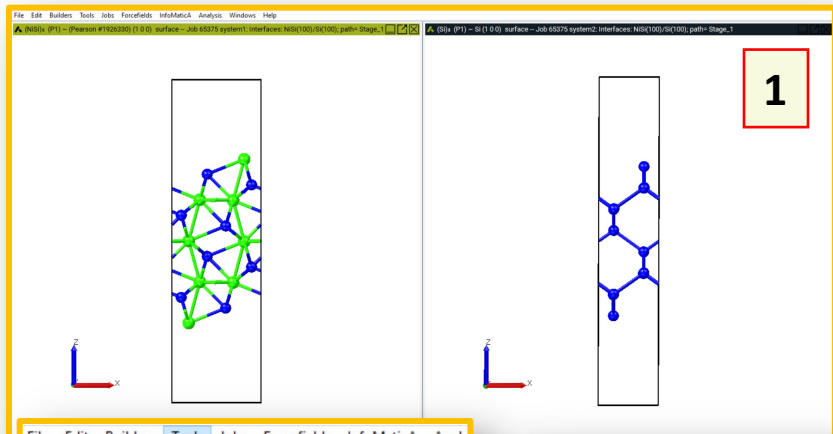
Next, an MLFF on Si/NiSi interface can be trained starting from Si+NiSi MLFF

MLFF for Si/NiSi interface: starting
from Si+NiSi MLFF

Si/NiSi (100) interface with *MedeA Interface Builder*

Build surface models

Retrieve and create an Interface model

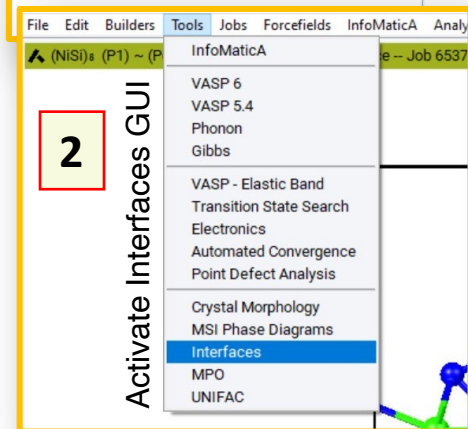


Materials Design Interfaces Builder: (Pearson #1926330) with Si (1 0 0) surface

ID	Identical Interfaces	nAtoms	Spacegroup	Area	dArea	A	dA	B	dB	theta	dTheta
1.1	Yes	88	P-1	87.24	-2.0	8.506	-1.4	10.862	0.5	109.2	1.4
1.2	Yes	88	P-1	87.24	-2.0	8.506	-1.4	10.862	0.5	109.2	1.4
1.3	Yes	88	P-1	87.24	-2.0	8.506	-1.4	10.862	0.5	109.2	1.4
1.4	Yes	88	P-1	87.24	-2.0	8.506	-1.4	10.862	0.5	109.2	1.4
1.5	Yes	88	P-1	87.24	-2.0	8.506	-1.4	10.863	-0.7	109.2	-2.1
1.6	Yes	88	P-1	87.24	-2.0	8.506	-1.4	10.863	-0.7	109.2	-2.1
1.7	Yes	88	P-1	87.24	-2.0	8.506	-1.4	10.863	-0.7	109.2	-2.1
1.8	Yes	88	P-1	87.24	-2.0	8.506	0.5	10.862	-2.8	109.2	-0.6
1.9	Yes	88	P-1	87.24	-2.0	8.506	-2.0	10.862	0.6	109.2	1.2
2.1	Yes	104	P-1	103.25	0.9	8.506	-1.4	12.220	1.7	96.6	-3.1

Interface cell in terms of original cell vectors of first system: $a' = a + 2b$, $b' = -2a + b$, of second system: $a' = 3b$, $b' = -2a + b$

Close



File Edit Builders Tools Jobs Forcefields InfoMaticA Analy

(NiSi)8 (P1) ~ (P)

InfoMaticA

e -- Job 6537

VASP 6

VASP 5.4

Phonon

Gibbs

VASP - Elastic Band

Transition State Search

Electronics

Automated Convergence

Point Defect Analysis

Crystal Morphology

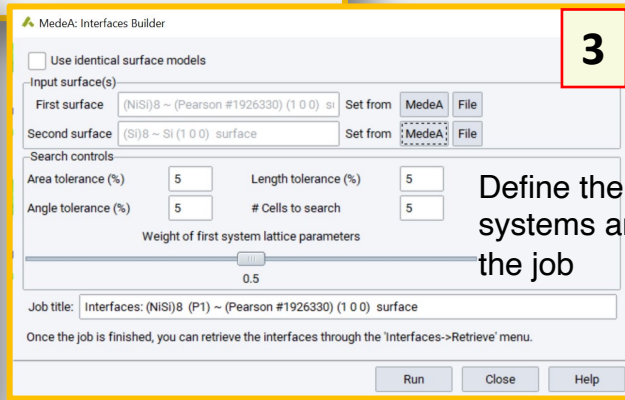
MSI Phase Diagrams

Interfaces

MPO

UNIFAC

Activate Interfaces GUI



MedeA: Interfaces Builder

Use identical surface models

Input surface(s)

First surface (NiSi)8 ~ (Pearson #1926330) (1 0 0) si Set from MedeA File

Second surface (Si)8 ~ Si (1 0 0) surface Set from MedeA File

Search controls

Area tolerance (%) 5 Length tolerance (%) 5

Angle tolerance (%) 5 # Cells to search 5

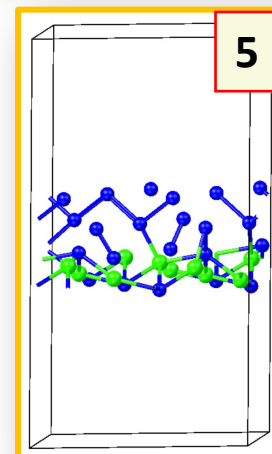
Weight of first system lattice parameters 0.5

Job title: Interfaces: (NiSi)8 (P1) ~ (Pearson #1926330) (1 0 0) surface

Once the job is finished, you can retrieve the interfaces through the 'Interfaces->Retrieve' menu.

Run Close Help

Define the two systems and run the job



Si/NiSi (100) interface

Train an MLFF on Si/NiSi interface *starting from MLFF trained on Si+NiSi*

Calculation Functional/Potential SCF DOS/Optic/Tensors Band Structure Advanced/Restart **Add to Input** Preview Input

Type of calculation Molecular Dynamics

Molecular Dynamics Parameters

Ensemble canonical (nVT)

Simulation time: 11000 fs

Time step: 2.0 fs

Trajectory file frequency: 1 steps

Temperature initial: 400.0 K

Temperature end: K

Nosé mass:

Continuation of job: ...

Involve machine-learned forcefield

Task Continue on-the-fly learning

Using forcefield of job: 65378

Properties

(Pseudo, difference, (Total, valence) charge

Interaction Functional Density functional

Calculation Functional/Potential SCF DOS/Optic/Tensors Band Structure Advanced/Restart **Input added** Preview Input

Additional Input Lines

ML_MB = 7500 → Increase maximum number of reference configurations for training

RANDOM_SEED = 60034400 0 0

to be non-mag

General Setup

Precision Normal

Increase planewave cutoff (cell optimizations)

Planewave cutoff (default): 245.345 eV

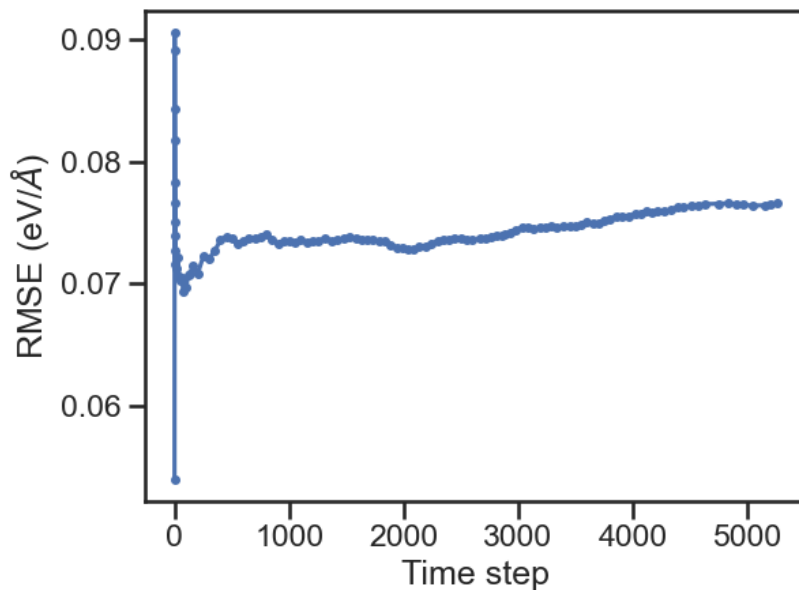
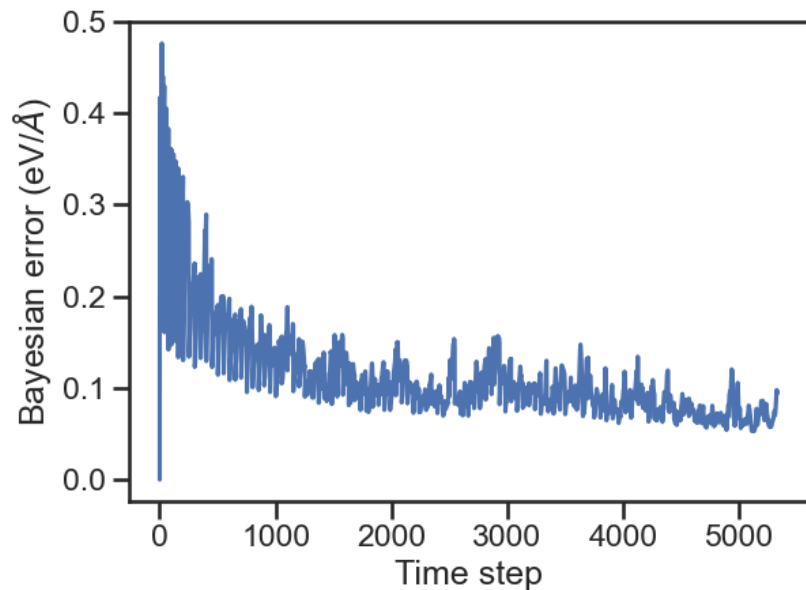
Planewave cutoff: 300 eV

Projection Real space

VASP version standard

Continue from the MLFF
trained on NiSi started from
the forcefield trained on Si

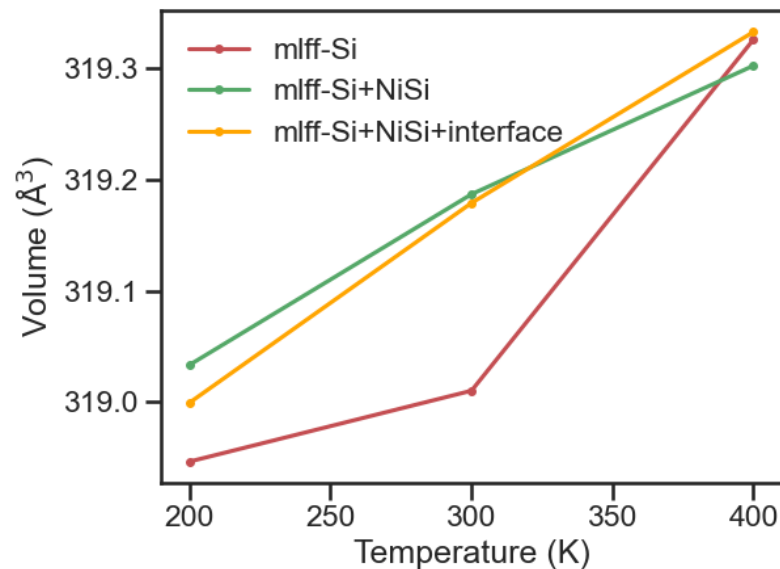
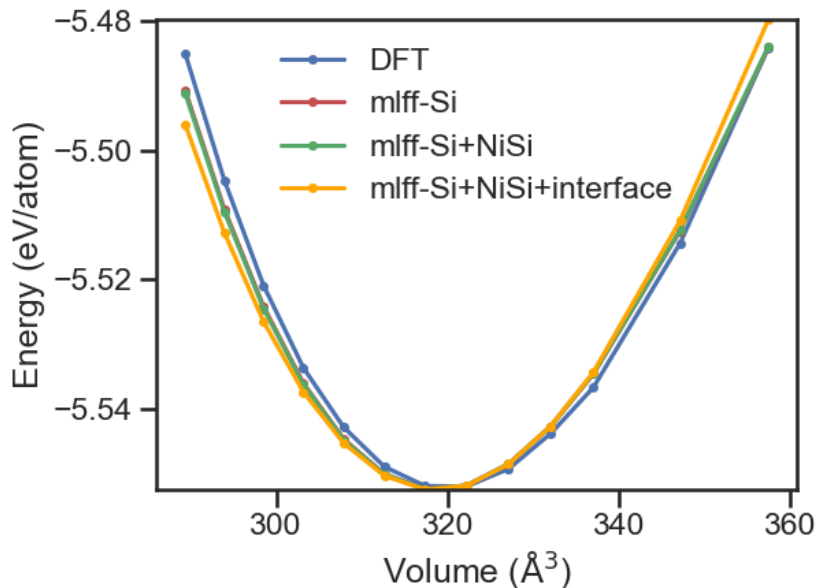
Si/NiSi(100) interface- Bayesian error and RMSE on atomic forces starting from MLFF of Si+NiSi



- 11ps, nPT, fixed cell shape (atom relaxation only), 300 eV cutoff, gamma-only point, 32-atom interface model
- Errors on forces slightly higher than previous MLFFs, due to complexity of the interface
- Possible ways to achieve better accuracy: train for longer than 10ps, more than 1 k-point in x-, and y-directions, use a thicker interface model
- Training time: ~9.5 hrs, 32 atoms, 11 ps, 12 cores

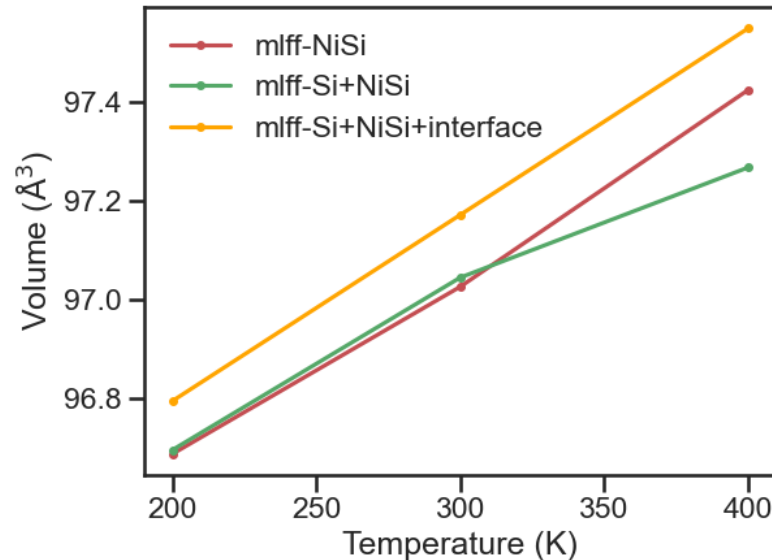
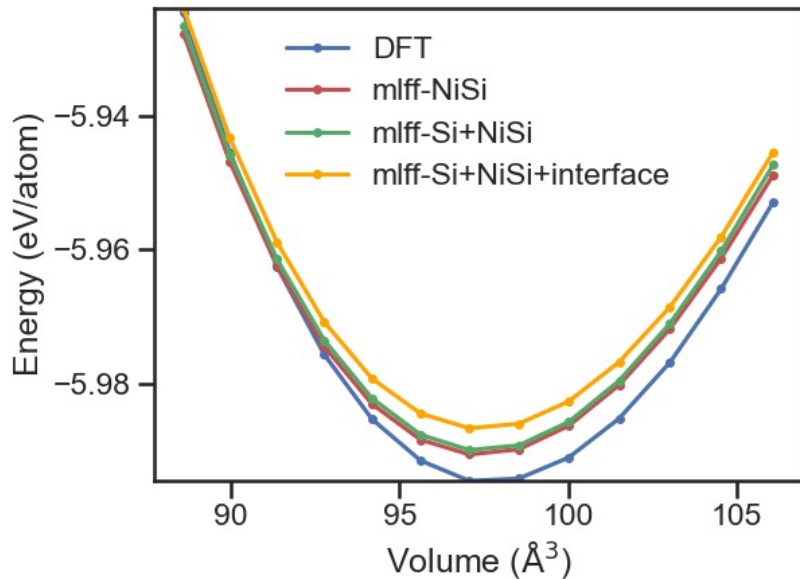
How does this combined Si+NiSi+interface MLFF perform for Si and NiSi properties?

Si: Si+NiSi+interface MLFF predicted volume-energy curve and thermal expansion



The combined Si+NiSi+interface retains the good agreement for volume-energy curves and behave similar to the Si+NiSi MLFF for thermal expansion

NiSi: Si+NiSi+interface MLFF predicted volume-energy curve and thermal expansion



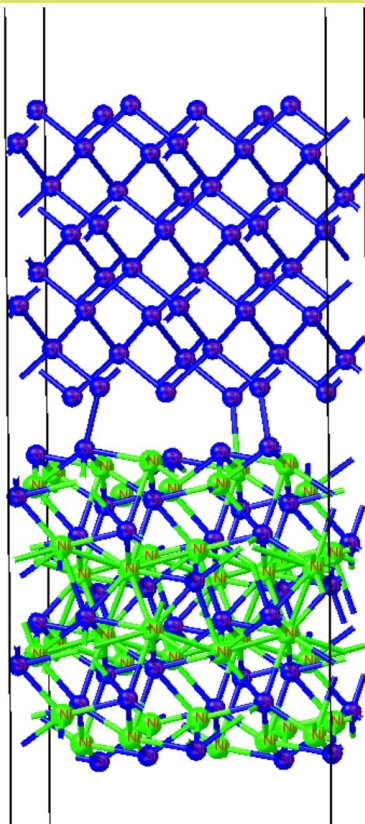
- Slight over-estimation of energies w.r.t DFT and other combined MLFFs, but all contained within 10 meV/atom
- Similar behavior for thermal expansion for all 3 MLFFs

Long MD simulation on Si/NiSi
interface with combined MLFF

Apply the Si+NiSi+interface MLFF on a larger interface model

Si/NiSi (100) interface, 128 atoms

nVT ensemble, 20ps, 400 K



Calculation	Functional/Potential	SCF	DOS/Optic/Tensors	Band Structure	Advanced/Restart	Add to Input	Preview Input
Type of calculation: Molecular Dynamics							
Molecular Dynamics Parameters							
Ensemble: canonical (nVT)							
Simulation time: 20000 fs							
Time step: 2.0 fs							
Trajectory file frequency: 100 steps							
Temperature initial: 400.0 K							
Temperature end: K							
Nosé mass:							
Continuation of job:							
<input checked="" type="checkbox"/> Involve machine-learned forcefield							
Task: Apply machine-learned forcefield							
Using forcefield of job: 68114							
Properties							
<input type="checkbox"/> (Pseudo, difference, spin) charge density							
<input type="checkbox"/> Total local potential							
<input type="checkbox"/> Electron localization function							
<input type="checkbox"/> Wave functions							
<input type="checkbox"/> Electric field gradients							
<input type="checkbox"/> Hyperfine parameters							
<input type="checkbox"/> Work function (surfaces only)							
<input type="checkbox"/> (Total, valence) charge density, Bader analysis							
<input type="checkbox"/> Band structure							
<input type="checkbox"/> Density of states							
<input type="checkbox"/> Optical spectra							
<input type="checkbox"/> Zone center phonons							
<input type="checkbox"/> Response tensors							
<input type="checkbox"/> NMR: chemical shifts							
<input type="checkbox"/> Energy of formation							
Solvation (for molecules or surfaces)							
<input type="checkbox"/> Apply solvation model							
External pressure: 0 GPa							
Charge state: 0 e							
External electrostatic field (molecules and surfaces): none							
Interaction							
Functional: Density functional							
DFT exchange-correlation: GGA-PBE							
Van der Waals: None							
Magnetism: Defined by model							
to be non-mag							
General Setup							
Precision: Normal							
<input type="checkbox"/> Increase planewave cutoff (cell optimizations)							
Planewave cutoff (default): 269.532 eV							
Planewave cutoff: 300 eV							
Projection: Real space							
VASP version: standard							

Apply MLFF trained on Si/NiSi interface started from the forcefield trained on Si+NiSi

Compute time: ~13 hrs, 128 atoms, 20 ps, 12 cores

Guidelines for MLFF training

- Use a large enough system to avoid volume fluctuations and to “fit” collective vibrations into the supercell, to be able to apply MLFF to a larger supercell
- Important to learn correct forces: accurate DFT settings, dense k-points, 30% higher plane-wave cutoff than default, appropriate electronic convergence algorithm for good electronic convergence
- Do not use too large time-steps, especially for light elements
- When using temperature ramping, be careful to stay in temperature regime where no phase transitions are induced
- Use nPT ensemble whenever possible – additional cell fluctuations increases robustness of the resulting forcefield (perform nVT and refine MLFF)
- Test nPT settings: atomic and lattice friction coefficients with **LANGEVIN_GAMMA** and **LANGEVIN_GAMMA_L** tags (“Add to Input” in MedeA VASP GUI), and Parrinello-Rahman mass
- Increase Bayesian threshold for force if needed: **ML_CTIFOR** (“Add to Input”); default is 0.002 eV/Å

MedeA VASP MLFF and MedeA MLPG

MedeA VASP MLFF

← complementary →

MedeA MLPG

- Both functionalities are machine-learned parameterizations of potential energy surfaces and are intended to calculate materials properties quickly with an accuracy of VASP
- In fact, VASP MLFF and SNAP MLP are both based on the Kernel Regression method
- However, MLPs (*SNAP and NNP*) are designed to work with much larger systems and with *LAMMPS*, while MLFFs are both trained and applied within VASP
- *MedeA MLPG* can use both VASP-MD trajectories and 0K calculated structures (distortions, defects, etc.), while VASP MLFF makes use of only MD trajectories for training

Relevant *MedeA* Modules

MedeA Environment (InfoMaticA and Advanced Builders)

MedeA VASP 6 (MLFF and DFT methods)

MedeA Interface Builder

MedeA HT-Launchpad (save an MD trajectory into structure list)

<https://www.materialsdesign.com/webinars/recorded>

Question and Answer Session



Dr. David Reith

Materials Design



Dr. Shubham Pandey

Materials Design



Dr. Xiaoli Liu

Materials Design

Announcements

ugm.materialsdesign.com

Next Week's MedeA Training

Thursday, October 27th



Dr. Marianna Yiannourakou

Materials Design



Dr. Jörg-Rütiger Hill

Materials Design

Next Week's Plenary Session

Tuesday, October 25th



Dr. Jozef Bicerano

Bicerano & Associates Consulting, LLC

Questions about Materials Design UGM

ugm@materialsdesign.com

Support Team

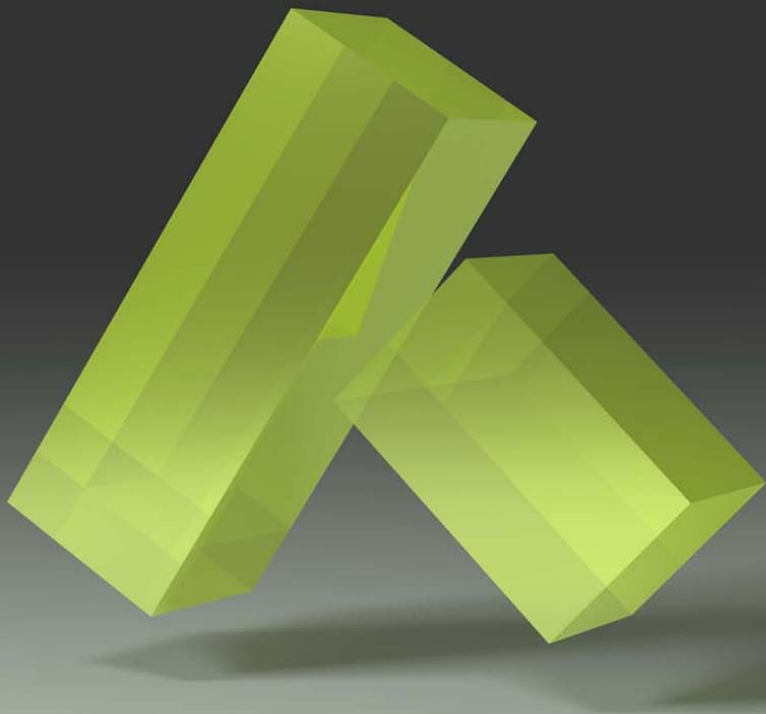
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